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Unified description of ${}^6\text{Li}$ structure and deuterium- ${}^4\text{He}$ dynamics with chiral two- and three-nucleon forces

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Prototype for the study of weakly bound projectiles colliding on stable targets, the scattering of deuterium (d) on ${}^4\text{He}$ (α) is an important milestone in the search for a fundamental understanding of low-energy reactions. At the same time, it is also important for its role in the Big-bang nucleosynthesis of ${}^6\text{Li}$ and applications in the characterization of deuterium impurities in materials. We present the first *ab initio* study of the ${}^6\text{Li}$ ground state and d - ${}^4\text{He}$ elastic scattering using two- and three-nucleon forces derived within the framework of chiral effective field theory. The six-nucleon bound-state and scattering observables are calculated by means of the no-core shell model with continuum and are compared to available experimental data. We analyze the influence of the dynamic polarization of the deuterium and of the chiral three-nucleon force, and examine the role of the continuum degrees of freedom in shaping the low-lying spectrum of ${}^6\text{Li}$. We find that the adopted Hamiltonian overderbinds ${}^6\text{Li}$ by 15 KeV and overestimates the excitation energy of the first 3^+ state by 340 KeV. The bulk of the computed differential cross section is in good agreement with data and the three-nucleon force plays an essential role in the zero-energy limit.

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Introduction. Lithium-6 (${}^6\text{Li}$) is a weakly-bound stable nucleus that breaks into an ${}^4\text{He}$ (or α particle) and a deuteron (d) at the excitation energy of 1.4743 MeV [1]. Until now out of reach of *ab initio* techniques, a complete unified treatment of the bound and continuum properties of this system is desirable to further our understanding of the fundamental interactions among nucleons, but also to inform the evaluation of low-energy cross sections relevant to applications. Notable examples are the ${}^2\text{H}(\alpha, \gamma){}^6\text{Li}$ radiative capture (responsible for the Big-bang nucleosynthesis of ${}^6\text{Li}$) and the ${}^2\text{H}(\alpha, d){}^4\text{He}$ cross section used in the characterization of deuteron concentrations in thin films. Well known experimentally, the low-lying resonances of ${}^6\text{Li}$ have been shown to present significant sensitivity to three-nucleon ($3N$) interactions in *ab initio* (i.e., from first principles) calculations that treated them as bound states [2–4]. However, this approximation is well justified only for the narrow 3^+ first excited state, and no information about the widths was provided. At the same time, the only *ab initio* study of d - ${}^4\text{He}$ scattering [5] was based on a nucleon-nucleon (NN) Hamiltonian and did not take into account the swelling of the α particle due to the interaction with the deuteron.

As demonstrated in a study of the unbound ${}^7\text{He}$ nucleus, the *ab initio* no-core shell model with continuum (NCSMC) [6, 7] is an efficient many-body approach to nuclear bound and scattering states alike. Initially developed to compute nucleon-nucleus collisions starting from a two-body Hamiltonian, this technique has been later extended to include $3N$ forces and successfully applied to make predictions of elastic scattering and recoil of protons off ${}^4\text{He}$ [8] and to study continuum and $3N$ -force effects on the energy levels of ${}^9\text{Be}$ [9]. We have now

developed the NCSMC formalism to describe more challenging deuterium-nucleus collisions, and as a first application, we present in this Letter a study of the ${}^6\text{Li}$ ground state (g.s.) and d - ${}^4\text{He}$ elastic scattering using $NN + 3N$ forces derived within the framework of chiral effective field theory.

Approach. We cast the microscopic ansatz for the ${}^6\text{Li}$ wave function in the form of a generalized cluster expansion

$$|\Psi^{J\pi T}\rangle = \sum_{\lambda} c_{\lambda} |{}^6\text{Li } \lambda J^{\pi T}\rangle + \sum_{\nu} \int dr r^2 \frac{\gamma_{\nu}(r)}{r} \mathcal{A}_{\nu} |\Phi_{\nu r}^{J\pi T}\rangle, \quad (1)$$

where J, π and T are respectively total angular momentum, parity and isospin, $|{}^6\text{Li } \lambda J^{\pi T}\rangle$ represent square-integrable energy eigenstates of the ${}^6\text{Li}$ system, and

$$|\Phi_{\nu r}^{J\pi T}\rangle = \left[(|{}^4\text{He } \lambda_{\alpha} J_{\alpha}^{\pi_{\alpha}} T_{\alpha}\rangle |{}^2\text{H } \lambda_d J_d^{\pi_d} T_d\rangle \right]^{(sT)} Y_{\ell}(\hat{r}_{\alpha,d}) \times \frac{\delta(r - r_{\alpha,d})}{r T_{\alpha,d}} \quad (2)$$

are continuous basis states built from a ${}^4\text{He}$ and a ${}^2\text{H}$ nuclei whose centers of mass are separated by the relative coordinate $\vec{r}_{\alpha,d}$, and that are moving in a $2s+1\ell_J$ partial wave of relative motion. The translationally-invariant compound, target and projectile states (with energy labels $\lambda, \lambda_{\alpha}$ and λ_d , respectively) are all obtained by means of the no-core shell model (NCSM) [10–12] using a basis of many-body harmonic oscillator (HO) wave functions with frequency $\hbar\Omega$ and up to N_{max} HO quanta above the lowest energy configuration. The index ν collects the quantum numbers $\{{}^4\text{He } \lambda_{\alpha} J_{\alpha}^{\pi_{\alpha}} T_{\alpha}; {}^2\text{H } \lambda_d J_d^{\pi_d} T_d; s\ell\}$ associated with the continuous basis states of Eq. (2), and

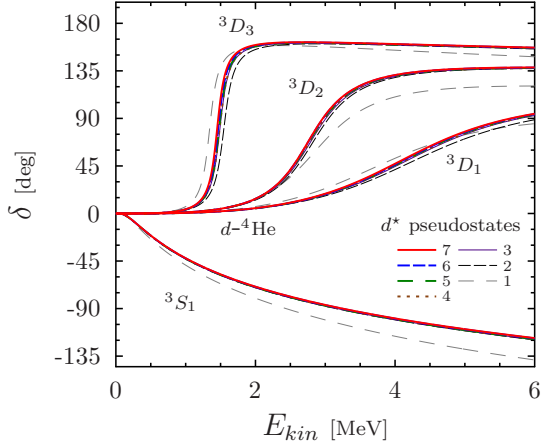


FIG. 1. (Color online) Computed d - ${}^4\text{He}$ S - and D -wave phase shifts at $N_{\text{max}} = 9$ and $\hbar\Omega = 20$ MeV, obtained including fifteen square-integrable ${}^6\text{Li}$ eigenstates, as a function of the number of ${}^2\text{H}$ states (up to seven) in the 3S_1 – 3D_1 , 3D_2 and 3D_3 – 3G_3 channels. The two-body part of the SRG-evolved $N^3\text{LO}$ NN potential (NN -only) with $\Lambda = 2.0 \text{ fm}^{-1}$ was used.

the operator (with $P_{i,j}$ exchanging particles i and j)

$$\mathcal{A}_\nu = \frac{1}{\sqrt{15}} \left(1 - \sum_{i=1}^4 \sum_{j=5}^6 P_{i,j} + \sum_{i<j=1}^4 P_{i,5} P_{j,6} \right),$$

ensures its full antisymmetrization. Finally, the unknown discrete coefficients, c_λ , and the continuous amplitudes of relative motion, $\gamma_\nu(r)$ are obtained by solving the six-body Schrödinger equation in the Hilbert space spanned by the basis states $|{}^6\text{Li} \lambda J^\pi T\rangle$ and $\mathcal{A}_\nu |\Phi_{\nu r}^{J^\pi T}\rangle$ [6, 7]. The elements of the scattering matrix are then obtained from matching the solutions of Eq. (1) with the known asymptotic behavior of the wave function using an extension of the microscopic R -matrix theory [13, 14].

The deuteron is only bound by 2.224 MeV. For relative kinetic energies (E_{kin}) above this threshold, the d - ${}^4\text{He}$ scattering problem is of a three-body nature (until the breakup of the tightly bound ${}^4\text{He}$, that is). Below, the virtual scattering to the energetically closed ${}^4\text{He}+p+n$ channels accounts for the distortion of the projectile. Here we address this by discretizing the continuum of ${}^2\text{H}$ in the 3S_1 – 3D_1 , 3D_2 and 3D_3 – 3G_3 channels identified in our earlier study of Ref. [5]. At the same time, the coupling of fifteen (among which two 1^+ , two 2^+ , and one 3^+) square-integrable six-body eigenstates of the composite system also contribute to the description of the deuteron distortion. More importantly, they address the swelling of the α particle [8], of which we only include the g.s. in Eq. (2). The typical convergence behavior of our computed d - ${}^4\text{He}$ phase shifts with respect to the number of deuteron pseudostates (or d^* , with $E_{d^*} > 0$) included in Eq. (2) is shown in Fig. 1. Stable results are found with as little as three deuteron states per channel. This

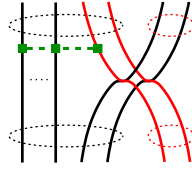


FIG. 2. (Color online) Diagrammatic representation of one of the $3N$ -force matrix elements between basis states of Eq. (2).

is a strong reduction of the d^* influence with respect to the more limited study of Ref. [5], lacking the coupling of square-integrable ${}^6\text{Li}$ eigenstates. Nonetheless, above the ${}^2\text{H}$ breakup threshold, our approach is approximated and a rigorous treatment would require the more complicated task of including three-cluster basis states [15] in the ansatz of Eq. (1).

The treatment of $3N$ forces within the NCSMC formalism to compute deuteron-nucleus collisions involves major technical and computational challenges. The first is the derivation and calculation of the matrix elements between the continuous basis states of Eq. (2) of seven independent $3N$ -force terms, five of which involve the exchange of one or two nucleons belonging to the projectile with those of the target. A typical example is the diagram of Fig. 2, which for the present application corresponds to $\langle \Phi_{\nu' r'}^{J^\pi T} | P_{3,5} P_{4,6} V_{123}^{3N} | \Phi_{\nu r}^{J^\pi T} \rangle$, with V_{123}^{3N} the $3N$ interaction among particles 1, 2 and 3. To calculate this contribution, we need the four-nucleon density matrix of the target. For ${}^4\text{He}$, this can be precomputed and stored in a factorized form [5, 16]. An additional difficulty, already mentioned in Ref. [16], involves the exorbitant number of input $3N$ force matrix elements (see Fig. 1 of Ref. [17]), which we have to limit by specifying a maximum three-nucleon HO model space size $E_{3\text{max}}$. To minimize the effects of such truncation we have included $3N$ -force matrix elements up to $E_{3\text{max}} = 17$. Finally, the contribution of the $3N$ forces to the coupling between the discrete and continuous portion of our basis is computationally less demanding and decomposes into the two terms $\langle {}^6\text{Li} \lambda J^\pi T | V_{346}^{3N} | \Phi_{\nu r}^{J^\pi T} \rangle$ and $\langle {}^6\text{Li} \lambda J^\pi T | V_{456}^{3N} | \Phi_{\nu r}^{J^\pi T} \rangle$.

Results. We adopt a Hamiltonian based on the chiral $N^3\text{LO}$ NN interaction of Ref. [20] and $N^2\text{LO}$ $3N$ force of Ref. [21], constrained to provide an accurate description of the $A=2$ and 3 [22] systems. These interactions are additionally softened by means of a unitary transformation that decouples high- and low-momentum components of the Hamiltonian, working within the similarity renormalization group (SRG) method [23–26]. To minimize the occurrence of induced four-nucleon forces, we work with the SRG momentum scale $\Lambda = 2.0 \text{ fm}^{-1}$ [16, 25, 26]. All calculations are carried out using the ansatz of Eq. (1) with fifteen discrete eigenstates of the ${}^6\text{Li}$ system and continuous d - ${}^4\text{He}$ (g.s.) binary-cluster states with up to seven deuteron pseudostates in the 3S_1 – 3D_1 , 3D_2 and 3D_3 – 3G_3 channels. Similar to our earlier study of d - ${}^4\text{He}$ scattering [5] [which was performed with a softer NN interaction but in a model space spanned only by the continuous basis states of Eq. (2)], we approach convergence

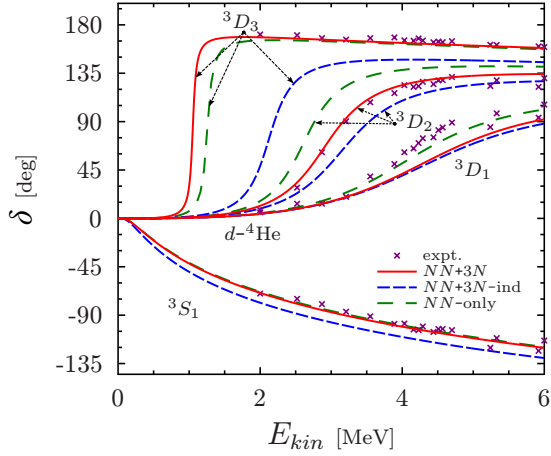


FIG. 3. (Color online) S - and D -wave d - ^4He phase shifts computed with the NN -only, $NN+3N$ -ind and $NN+3N$ Hamiltonians (lines) compared to those extracted from R -matrix analyses of data [18, 19] (symbols). More details in the text.

for the HO expansions at $N_{\text{max}} = 11$. For the HO frequency we adopt the value of 20 MeV around which the ^6Li g.s. energy calculated within the square-integrable basis of the NCSM becomes nearly insensitive to $\hbar\Omega$ [4].

We start by discussing the influence of $3N$ forces – those induced by the SRG transformation of the NN potential ($NN+3N$ -ind) as well as those initially present in the chiral Hamiltonian ($NN+3N$). In Fig. 3 we compare our computed d - ^4He S - and D -wave phase shifts with those of the R -matrix analyses of Refs. [18, 19]. The results based on the two-body part of the evolved NN force (NN -only) compare well with those of Ref. [5] (obtained with a softer potential) and, except for the splitting between the 3D_3 and 3D_2 resonances, with experiment. Once the SRG unitary equivalence is restored via the induced $3N$ force, the resonance centroids are systematically shifted to higher energies. By contrast, the agreement with data is much improved in the $NN+3N$ case and, in particular, the splitting between the 3D_3 and 3D_2 partial waves is comparable to the measured one.

TABLE I. Absolute g.s. energies of ^6Li using the $NN + 3N$ -ind and $NN + 3N$ Hamiltonians compared to experiment. The error estimates quoted in the extrapolated NCSM results include uncertainties due to the SRG evolution of the Hamiltonian and $\hbar\Omega$ dependence [4].

$E_{\text{g.s.}}$ [MeV]	$NN + 3N$ -ind	$NN + 3N$
NCSM ($N_{\text{max}} = 10$)	-26.56	-30.84
NCSM ($N_{\text{max}} = 12$)	-27.27	-31.52
NCSM (extrapolation [28])	-28.0(3)	-32.2(3)
NCSMC ($N_{\text{max}} = 10$)	-28.17	-32.01
Expt. [1, 29]	-31.99	

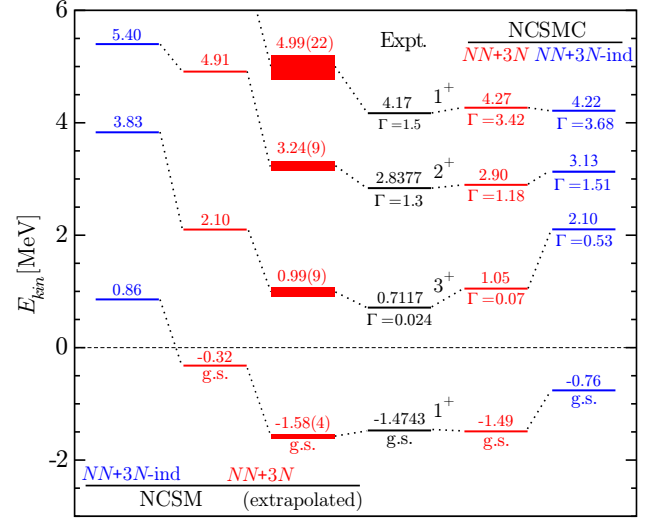


FIG. 4. (Color online) Ground-state energy and low-lying ^6Li positive-parity $T = 0$ resonance parameters extracted [27] from the phase shifts of Fig. 3 (NCSMC) compared to the evaluated centroids and widths (indicated by Γ) of Ref. [1] (Expt.). Also shown on the left-hand-side are the best ($N_{\text{max}} = 12$) and extrapolated [28] NCSM energy levels. The zero energy is set to the respective computed (experimental) d - ^4He breakup thresholds. Absolute g.s. energies can be found in Table I.

In Fig. 4, the resonance centroids and widths extracted [27] from the scattering phase shifts of Fig. 3 (shown on the right) are compared with experiment as well as with more traditional approximated energy levels (shown on the left) obtained within the NCSM by treating the ^6Li excited states as bound states. In terms of excitation energies relative to the g.s., in both calculations (i.e., with or without continuum effects) the chiral $3N$ force affects mainly the splitting between the 3^+ and 2^+ states, and to a lesser extent the position of the first excited state. Sensitivity to the chiral $3N$ force is also seen in the widths of the NCSMC resonances, which tend to become narrower (in closer agreement with experiment) when this force is present in the initial Hamiltonian. Overall, the closest agreement with the observed spectrum is obtained with the $NN+3N$ Hamiltonian working within the NCSMC, i.e. by including the continuum degrees of freedom. Compared to the best ($N_{\text{max}} = 12$) NCSM values, all resonances are shifted to lower energies commensurately with their distance from the d - ^4He breakup threshold. For the 3^+ , which is a narrow resonance, the effect is not sufficient to correct the slight overestimation in excitation energy already observed in the NCSM calculation. This and the ensuing underestimation of the splitting between the 2^+ and 3^+ states point to remaining deficiencies in the adopted $3N$ force model, particularly concerning the strength of the spin-orbit interaction.

As highlighted in Fig. 4, the inclusion of the d - ^4He

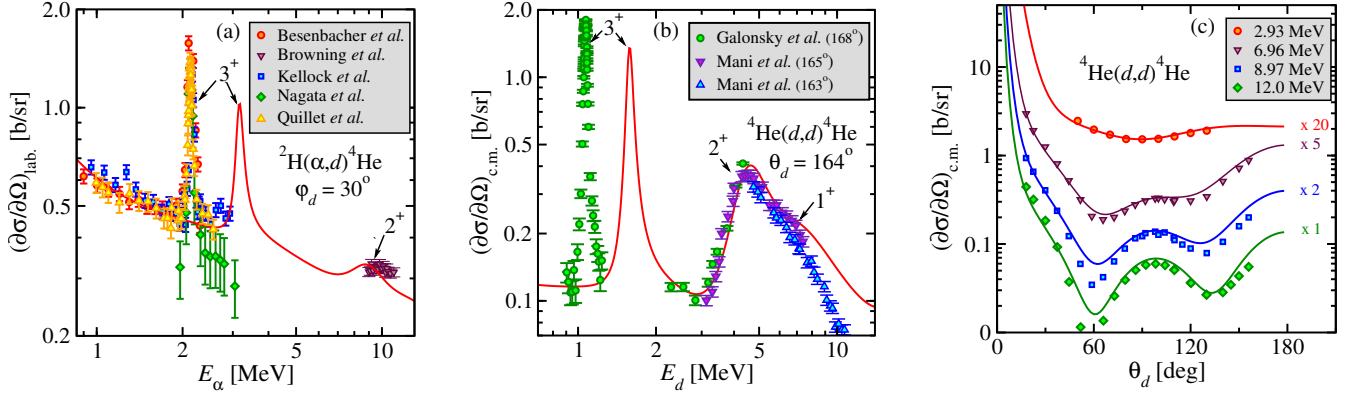


FIG. 5. (Color online) Computed (a) ${}^2\text{H}(\alpha, d){}^4\text{He}$ laboratory-frame and (b) ${}^4\text{He}(d, d){}^4\text{He}$ center-of-mass frame angular differential cross sections (lines) using the $NN+3N$ Hamiltonian at the deuteron recoil and backscattered angles of, respectively, $\varphi_d = 30^\circ$ and $\theta_d = 164^\circ$ as a function of the laboratory helium (E_α) and deuteron (E_d) incident energies, compared with data (symbols) from Refs. [30–36]. In panel (c), calculated (lines) and measured (symbols) center-of-mass angular distributions at $E_d = 2.93, 6.96, 8.97$ [37], and 12 MeV [38] are scaled by a factor of 20, 5, 2, and 1, respectively. All positive- and negative-parity partial waves up to $J = 3$ were included in the calculations.

binary-cluster states of Eq. (2) results also in additional binding for the 1^+ ground state. This can be understood as stemming from a more efficient description of the clusterization of ${}^6\text{Li}$ into a deuteron and an α particle at long distances, which is harder to describe within a finite HO model space, or – more simply – from the increased size of the many-body model space. Indeed, as shown in Fig. 4 and in Table I for the absolute value of the ${}^6\text{Li}$ g.s. energy, extrapolating to $N_{\text{max}} \rightarrow \infty$ [28] brings the NCSM results in good agreement with the NCSMC, particularly for bound states and narrow resonances. However, while the extrapolation procedure yields comparable energies, only the NCSMC wave functions present the correct asymptotic, which for the g.s. is a Whittaker function. This will be essential for the description of the ${}^2\text{H}(\alpha, \gamma){}^6\text{Li}$ radiative capture. Further, based on the extrapolated NCSM energies, one could erroneously conclude that the measured splitting between 2^+ and 3^+ state is reproduced with the $NN+3N$ Hamiltonian. Conversely, the square-integrable $|{}^6\text{Li} \lambda J^\pi T\rangle$ components of the ansatz (1) are essential for achieving an efficient description of the short-range six-body correlations, and address the polarization of the ${}^4\text{He}$ core. Describing such correlations exclusively within continuous basis states of the type of Eq. (2) would require the computationally unfeasible inclusion of a large number of ${}^4\text{He}$ excited states.

Next, in Figs. 5(a) and 5(b), respectively, we compare the ${}^2\text{H}(\alpha, d){}^4\text{He}$ deuteron elastic recoil and ${}^4\text{He}(d, d){}^4\text{He}$ deuteron elastic scattering differential cross sections computed using the $NN+3N$ Hamiltonian in the largest model space ($N_{\text{max}} = 11$) to the measured energy spectra of Refs. [30–36]. Aside from the position of the 3^+ resonance, the calculations are in fair agreement with experiment, particularly in the low-energy region of interest for the Big-bang nucleosynthesis of ${}^6\text{Li}$, where we reproduce the data of Besenbacher *et al.* [30] and those

of Quillet *et al.* [34]. The 500 KeV region below the resonance in Fig. 5(a) is also important for material science, where the elastic recoil of deuterium knocked by incident α particles is used to analyze the presence of this element. At higher energies, near the 2^+ and 1^+ resonances, the computed cross section at the center-of-mass deuteron scattering angle of $\theta_d = 164^\circ$ reproduces the data of Galonsky *et al.* [35] and Mani *et al.* [36], while we find slight disagreement with the data of Ref. [31] in the elastic recoil configuration at the laboratory angle of $\varphi_d = 30^\circ$. At even higher energies, the measured cross section of Fig. 5(b) lies below the calculated one. This is due in part to the overestimated width of the 1_2^+ state, which is twice as large as in experiment. At the same time, higher partial waves ($J > 3$) not considered here (the accurate calculation of which would require $3N$ -force matrix elements beyond $E_{3\text{max}} = 17$), become somewhat more important at these energies. The overall good agreement with experiment is also corroborated by Fig. 5(c), presenting ${}^4\text{He}(d, d){}^4\text{He}$ angular distributions in the $2.93 \leq E_d \leq 12.0$ MeV interval of deuteron incident energies. In particular, the theoretical curves reproduce the data at $E_d = 2.93$ and 6.96 MeV, while some deviations are visible at the two higher energies, in line with our previous discussion. Nevertheless, in general the present results including $3N$ forces provide a much more realistic description of the scattering process than our earlier study of Ref. [5]. Finally, while an $N_{\text{max}} = 13$ calculation (currently out of reach) may change the present picture somewhat, we expect that the differences with respect to the present results would not be substantial, particularly concerning the description of the narrow 3^+ resonance. Indeed, much as in the case of the g.s. energy, here the NCSMC centroid is in good agreement with the NCSM extrapolated value, 0.99(9) MeV.

Conclusions. We presented the first application of the NCSMC formalism for a reaction involving a two-nucleon projectile. In this *ab initio* calculation of d - ^4He elastic scattering, we illustrated the importance of the coupling to square-integrable ^6Li states and of the three-nucleon force. We used data for deuterium backscattering and recoil cross sections of interests to ion beam spectroscopy to validate our calculations and found a good agreement in particular at low energy. The overestimation by about 340 keV of the position of the 3^+ state is an indication of remaining deficiencies of the nuclear Hamiltonian employed here. This work sets the stage for the first *ab initio* study of the $^2\text{H}(\alpha, \gamma)^6\text{Li}$ radiative capture, and is a stepping stone in the calculation of the deuterium-tritium fusion with the chiral $NN + 3N$ Hamiltonian, currently in progress.

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